Origins of the Equations Describing Magnetization Dynamics

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Introduction

This report outlines steps in deriving the Bloch Equation, beginning from a simple classical model of a charged particle placed in a uniform magnetic field, and applying principles of quantum mechanics to derive, from the energy equation of the classical model, the two-component Schrödinger Equation describing the interaction of a proton with external magnetic fields. The off-diagonal entries of the Bloch equation matrix are then derived by taking the time derivative of the expectation values of the solutions of the Schrödinger Equation (the spinors) that describe the tissue protons. Derivations of the Boltzmann distribution which determines the thermal equilibrium magnetization, and of the mechanisms of magnetization relaxation, are also described to complete the entries of the Bloch Equation. An intuitive understanding of the proton gyromagnetic ratio, and of the physical origin of the Nuclear Magneton fundamental constant, is also obtained from the simple classical model.

Quantum mechanical model of the proton

This section presents the typical quantum mechanical description of the proton and its interaction with external magnetic fields. Here, the basic equations are simply written down and asserted to be accurate representations of the proton's experimental behavior. This section is provided mainly to serve as a reference to the basic equations; it should **not** be regarded as a foundation for the remaining sections of the report. In later sections, this report will focus on the application of the principles of quantum mechanics to *derive* these basic equations from a simple classical model of the proton.

Intrinsic spin and intrinsic angular momentum

Pauli postulated that nuclei possess an intrinsic angular momentum $\mathbf{J}$ and an associated intrinsic magnetic moment $\boldsymbol{\mu}$. The relationship between this angular momentum and this magnetic moment is $\boldsymbol{\mu} = 2\pi\gamma\mathbf{J}$ where γ is the gyromagnetic ratio (in units of cycles/unit-time/unit-field, e.g. Hz/Tesla). The intrinsic spin $\mathbf{I}$ of a nucleus determines the number of distinct energy levels of the nucleus when it is placed in an external magnetic field. The intrinsic spin is related to the intrinsic angular momentum by $\mathbf{J} = \hbar\mathbf{I}$ where $\hbar$ is Planck's constant. In a magnetic field taken to be aligned with the z axis of the laboratory coordinate system, the z component of intrinsic spin for a spin ½ particle such as a proton has two possible energy states, spin-up (aligned or parallel) and spin-down (anti-aligned or anti-parallel). The spin-up state is the low energy state, corresponding to $\mathbf{I}_z = 1/2$, and the spin-down state is the high energy state, corresponding to $\mathbf{I}_z = -1/2$.

The Larmor equation

The proton magnetic moment interacts with the applied external magnetic field and the component of the intrinsic spin along the direction of the main magnetic field determines the relative energy. The energy E of a classical particle with magnetic moment $\boldsymbol{\mu}$ in an external magnetic field $\mathbf{B}$ is given by the equation $E = -\boldsymbol{\mu}\cdot\mathbf{B}$. The energy for a quantum mechanical particle in an external magnetic field along the z direction, $\mathbf{B} = B_0\hat{\mathbf{z}}$, is found by substituting into that energy equation the intrinsic magnetic moment to yield $E = -2\pi\gamma\hbar\mathbf{I}_z B_0$. Consequently, the energy difference ΔE between the two spin states of the proton is $\Delta E = 2\pi\gamma\hbar B_0$. An electromagnetic field

oscillating at temporal frequency ω is composed of photons with quantized energy E in accordance with the Einstein relation $E = \hbar\omega$. An electromagnetic field can cause the proton to transition between its low energy and high energy spin states, if the photon energy matches the energy required for the transition. The required temporal frequency of the electromagnetic field is found by equating the photon energy $\hbar\omega$ with ΔE, and is given by the Larmor relation $\omega = 2\pi\gamma B_0$.

A simple classical model of the proton

Description of the model and interpretation of the gyromagnetic ratio

The classical model described in this section is the foundation and starting point for all of the remaining derivations in this report, and ending with the deviation of the Bloch equation. In this classical model, the proton is naively represented as a charged point particle with a mass m and charge e revolving at a constant radius $|\mathbf{r}|$ around an axis with velocity $\mathbf{v}$ and momentum $\mathbf{p} = m\mathbf{v}$. The angular momentum $\mathbf{L}$ of this system is $\mathbf{L} = \mathbf{r} \times \mathbf{p}$. In this simple model, $\mathbf{r}$ and $\mathbf{p}$ remain perpendicular, and the formula for angular momentum along the z direction is $L = m\,r\,v$ where v is the velocity magnitude and r is the radius. From classical electromagnetism, the magnetic moment along the z direction, denoted μ, is defined by the effective current of the revolving particle multiplied by the cross-sectional area πr^2 enclosed by the circular orbit. This magnetic moment is $\mu = i\,\pi r^2$, where i is the effective current of the particle. The current is $i = e/T$, where T is the time duration for the particle to traverse one orbit given by $T = 2\pi r/v$. Thus, $\mu = \left(ev/2\pi r\right)\pi r^2 = evr/2$, and with $\mu = 2\pi\gamma L$ implies $2\pi\gamma = e/2m$.

Derivation of the Nuclear Magneton

The theoretical value obtained for the proton gyromagnetic ratio using the formula above does not match the experimentally-derived value for the proton gyromagnetic ratio (see below). Perhaps, this result is not surprising given the naivety of the classical model. Nevertheless, this model and formula are used to define the Nuclear Magneton, a fundamental constant that appears in virtually all tables of "Fundamental Physics Constants". The Nuclear Magneton, denoted μ_N, is the value of the magnetic moment of the proton based on the classical model above, using the experimental proton mass m and unit charge e and with intrinsic spin $\mathbf{I}_z$ set to 1. Consequently, the formula used to calculate the Nuclear Magneton is $\mu_N = 2\pi\gamma\hbar = e\hbar/2m$. Typically in handbooks, the ratio μ/μ_N is given as the experimentally-derived value of the magnetic moment (e.g. 2.793 for proton). Similarly, an experimentally derived value of the gyromagnetic ratio can be reported as $2\pi\gamma$, and the theoretical value $e/2m$ may be identified as the gyromagnetic ratio of the Nuclear Magneton equal to $2\pi\gamma_N$. Inserting the proton mass and charge, and Planck's constant, yields $\mu_N = 5.0509\times10^{-27}$ Joules/Tesla and $\gamma_N = 7.622\times10^7$ Hz/Tesla. If the ratio μ/μ_N is given, then the experimentally-derived value for γ can be obtained using $\gamma = \gamma_N \left(\mu/\mu_N\right)/\mathbf{I}_z$.

Principles of Quantum mechanics

Particle wave duality: Wavefunctions and their interpretation

Protons, electrons, and other subatomic particles are often treated as classical particles (i.e., point masses moving with well defined position, momentum and energy, and obeying the laws of classical physics. However, these particles also exhibit properties characteristic of waves. The wave nature of the subatomic particle is conveyed by the de Broglie relation $\mathbf{p} = \hbar\mathbf{k}$ involving the classical momentum of the particle $\mathbf{p} = m\,\mathbf{v}$, and the wave number $\mathbf{k}$ (radians/unit distance) of a plane wave. The particle nature is conveyed by the Einstein relation $E = \sqrt{\left(\mathbf{p}\cdot\mathbf{p}\right)c^2 + \left(mc^2\right)^2}$ involving the particle energy E, the particle momentum $\mathbf{p}$, and the mass m, and where c is the speed of light. Photons, the particles associated with electromagnetic fields, have zero mass. In this case, the Einstein relation reduces to $E = pc$ where $p = |\mathbf{p}|$. Since the temporal frequency in radians/s of a wave with velocity c and wave number k is $\omega = kc$ where $k = |\mathbf{k}|$, it follows for particles with zero mass that $E = \hbar\omega$.

Plane-wave wavefunctions of "well-defined" energy and momentum

For freely moving particles (meaning that there is no potential field or force affecting the motion of the particles), wave-particle duality is represented by plane waves that have precisely defined, often referred to as "well-defined", energy and momentum. A plane wave is represented by $\psi(\mathbf{r},t) = \exp(i(\mathbf{k}\cdot\mathbf{r} - \omega t))$ where $\mathbf{r}$ represents the spatial coordinate and $\mathbf{k}$ is the direction of propagation, ω is the temporal frequency, and t is time. Using the Einstein and de Broglie relations, the plane wave representing the particle can be rewritten $\psi(\mathbf{r},t) = \exp(\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{r} - Et))$ yielding a wave description of a particle that has well defined energy E and momentum $\mathbf{p}$ as needed for the notion of a particle. This plane wave representation is a starting point for discussion of wavefunctions representing particles with more complicated quantum mechanical properties.

Derivation of differential equations for wavefunctions (the wave equations)

In classical physics, the equations of motion of point particles can be derived from the conservation equations involving energy E, momentum $\mathbf{p}$, angular momentum $\mathbf{L}$, and mass m of the particle. For example, the energy equation $E = \mathbf{p}\cdot\mathbf{p}/2m$ describes a non-relativistic classical point particle with energy E and momentum $\mathbf{p}$ traveling in free space without any influence of external forces. Using Hamilton's principle from classical mechanics, differential equations describing the motion of the point particle can be derived from the corresponding classical energy equation. In Quantum Mechanics, through a process of substituting scalar variables with corresponding differential operators, the classical energy and momentum conservation equations that describe the motion of classical point particles are converted into differential equations whose solutions are the wavefunctions describing the corresponding quantum mechanical particle with both wave and particle properties. These wavefunctions predict the unique behavior of the quantum-mechanical particle that is not predicted by the classical laws of motion.

The differential operators E_{op}, $\mathbf{p}_{op}$ and $\mathbf{r}_{op}$ that are used in the substitution have the unique property that when they act on plane waves with well-defined energy and momentum, they output the corresponding physical scalar or vector quantities E, $\mathbf{p}$ and $\mathbf{r}$, respectively. For example, the momentum operator $\mathbf{p}_{op}$ is proportional to the derivative with respect to $\mathbf{r}$, i.e., $\mathbf{p}_{op} = (\hbar/i)\partial/\partial\mathbf{r}$. Using the expression for the plane wave above it is seen that $\mathbf{p}_{op}\psi = \mathbf{p}\psi$. Likewise, the energy operator is proportional to the derivative with respect to t, i.e., $E_{op} = i\hbar\partial/\partial t$. Using the expression for the plane wave it is seen that $E_{op}\psi = E\psi$. With respect to operators that depend on location $\mathbf{r}$, no derivative operations are necessary, since the plane wave is considered to be function of $\mathbf{r}$, so $\mathbf{r}_{op}\psi = \mathbf{r}\psi$. Generally, functions that satisfy an operator equation for general operator $\mathbf{A}_{op}$ of the form $\mathbf{A}_{op}\psi = A\psi$ are called the eigenfunctions of operator $\mathbf{A}_{op}$, and for each eigenfunction, the scalar quantity A on the right side is referred to as the corresponding eigenvalue for that eigenfunction. The association of these specific differential operators with the physical quantities is a result of the so-called Correspondence Principle, which demands that the Quantum mechanical description of a physical system is consistent with the correct classical equations of motion in the various situations in which $\hbar$ is very small relative to other dimensions of the systems.

Operator substitution applied to the energy equation of a classical model of the hydrogen atom

The well-known Schrödinger differential equation for the hydrogen atom is obtained from the energy equation for a simple classical model of an electron in the electric field of a charged point nucleus. This fundamental differential equation leads to the electron orbital theory used in Chemistry. The energy equation for the particle in a potential field is given by $E = |\mathbf{p}|^2/2m - e/|\mathbf{r}|$, which is simply the sum of the kinetic and potential energies of the electron in the potential field of the nucleus. Using the differential operator substitutions, the differential equation $i\hbar\partial\psi(\mathbf{r},t)/\partial t = -(\hbar^2/2m)\nabla^2\psi(\mathbf{r},t) - (e/|\mathbf{r}|)\psi(\mathbf{r},t)$ is found for which the solutions $\psi(\mathbf{r},t)$ are wavefunctions describing the electrons in the potential field of the nucleus. The solutions to this differential equation are denoted by $\psi_{n,l,m}(\mathbf{r},t)$ and are given by the product of radial functions $R_n(\mathbf{r})$ and spherical harmonic functions $Y_{l,m}(\theta,\varphi)$. $\psi_{n,l,m}(\mathbf{r},t)$ represent the well known electron orbitals of well-defined energy (i.e., the s,p,d,f, etc. orbitals and

indexed by integer n) and of well-defined total angular momentum (indexed by integer l) and of well-defined z component of angular momentum (indexed by m).

Wavefunction interpretation

A fundamental postulate of quantum mechanics states that the squared modulus of a wavefunction describing a particle, given by $\left|\psi\left(\mathbf{r},t\right)\right|^{2}$, is the probability density that the particle will be measured at position $\mathbf{r}$ at time t, if the appropriate experiment is done to determine the particles position at time t. This postulate is confirmed by numerous experiments that reveal the interference patterns of wavefunctions and the associated particle densities predicted by those patterns. The probability density interpretation demands that the wavefunction is normalized, in the sense that the integral of a probability density function over all possible $\mathbf{r}$ locations of the particle must equal one. Assuming that possible locations of the particle are restricted to a volume V, the normalization condition reads $\int_{V}\left|\psi\left(\mathbf{r},t\right)\right|^{2}d\mathbf{r}=1$.

Expectation values of wavefunctions

The so-called expectation value $\left\langle \mathbf{A}_{op}\right\rangle$ for a quantum mechanical operator $\mathbf{A}_{op}$ is given by $\left\langle \mathbf{A}_{op}\right\rangle =\int_{v}\psi^{\dagger}\left(\mathbf{r},t\right)\mathbf{A}_{op}\psi\left(\mathbf{r},t\right)d\mathbf{r}$. This expression is equivalent to the weighted average of the variable associated with the operator $\mathbf{A}_{op}$ representing that physical parameter (such as momentum), weighted by the probability density function $\left|\psi\left(\mathbf{r},t\right)\right|^{2}$ for the wavefunction. It is important to understand the meaning of the expectation value in the context of performing experiments on a quantum mechanical particle. Suppose that you have prepared a quantum mechanical particle such that it is represented by wavefunction $\psi\left(\mathbf{r},t\right)$. It is critical to understand that the expectation value is not the value that one expects to obtain in a single measurement of this physical parameter. Instead, the expectation value is the average value of the measurements obtain when the experiment is done over and over again on a large number of identically prepared particles. If precisely the same experiment is done on these different but identically prepared particles, a different value for the physical parameter would be obtained in each experiment. Furthermore, a histogram of the obtained values would match the probability density function $\left|\psi\left(\mathbf{r},t\right)\right|^{2}$, and the number obtained by averaging the values obtained from all of the experiments would be equal to the expectation value. This result is distinctly different from the result that would be obtained from a large number of classical particles prepared in the same state. In that case, every particle would give the same value for the physical parameter.

The expectation value formula above is applicable with any normalized wavefunction describing a particle or particles in the physical system. In particular, for particles represented by simple plane waves with well-defined energy and momentum, it can be seen directly that the formula extracts the value of the momentum from the plane wave description. For example, the momentum operator $\mathbf{p}_{op}$ extracts a factor of $\mathbf{p}$ from the complex exponential into the integrand, yielding the x-independent value $\mathbf{p}$ that can be pulled out of the integral. Proper wavefunction normalization leads to the result $\left\langle \mathbf{p}_{op}\right\rangle =1/V\int_{V}d\mathbf{r}\exp\left(-i/\hbar\left(\mathbf{p}\cdot\mathbf{r}-Et\right)\right)\left(\hbar/i\ \partial/\partial\mathbf{r}\right)\exp\left(i/\hbar\left(\mathbf{p}\cdot\mathbf{r}-Et\right)\right)=\mathbf{p}$.

A wavefunction with a "well-defined" physical parameter describes a physical system in which the same numerical value for that physical parameter is obtained whenever a measurement of that parameter is made. Each such wavefunction is an eigenfunction of the operator for that physical parameter, and the expectation value of that wavefunction will be equal to its corresponding eigenvalue. For example, for the momentum operator above, we see that $\mathbf{p}_{op}\psi=\left(\hbar/i\right)\partial/\partial\mathbf{r}\exp\left(i/\hbar\left(\mathbf{p}\cdot\mathbf{r}-Et\right)\right)=\mathbf{p}\psi=\left\langle \mathbf{p}_{op}\right\rangle \psi$, meaning that the plane wave represents a wavefunction of the physical system with a well-defined momentum.

Principles of quantum mechanics applied to the classical model of the proton

Operator substitution applied to the energy equation for a particle in an external magnetic field

The energy of interaction between a classical particle possessing a magnetic moment and an external magnetic field is equal to $E = -\mathbf{\mu} \cdot \mathbf{B}$. A proton with a magnetic moment has been modeled above as a point particle with mass m and charge e revolving around an axis in a magnetic field. In a classical system, the angular momentum (denoted here by $\mathbf{L}$ rather than $\mathbf{J}$ which will be reserved for the angular momentum of the quantum mechanical system) of this revolving particle is equal to $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, where $\mathbf{r}$ and $\mathbf{p}$ are the position and linear momentum of the particle. The magnetic moment is $\mathbf{\mu} = 2\pi \gamma_N \mathbf{L}$, where γ_N is the theoretically-derived gyromagnetic ratio for the model. Using the substitutions, the energy equation is converted to a differential equation with solution $\psi(\mathbf{r},t)$ given by $i\hbar \partial \psi(\mathbf{r},t)/\partial t = -2\pi\gamma_N (\mathbf{L}_{op} \cdot \mathbf{B}) \psi(\mathbf{r},t)$. The angular momentum operator, denoted $\mathbf{L}_{op}$, is found by taking the cross product of the position operator with the momentum operator given by $\mathbf{L}_{op} = \mathbf{r}_{op} \times \mathbf{p}_{op}$. In forming this operator, the order of the operators must be preserved, since the derivatives of $\mathbf{p}_{op}$ will act on the x, y, and z coordinates of the position operator $\mathbf{r} \equiv \mathbf{r}_{op}$. For example, the z component of $\mathbf{L}_{op}$ is given by $\mathbf{L}_{op,z} = x\, \mathbf{p}_{op,y} - y\, \mathbf{p}_{op,x} = \hbar/i\, (x\, \partial/\partial y - y\, \partial/\partial x)$.

The structure of the differential equation and wavefunction is revealed by choosing the external field $\mathbf{B}$ to be oriented in the z direction. For this case, the differential equation simplifies to $\partial \psi(\mathbf{r},t)/\partial t = -\omega(x\, \partial/\partial y - y\, \partial/\partial x)\psi(\mathbf{r},t)$ where $\omega = 2\pi\gamma_N \mathbf{B}_z$ is identified as the Larmor frequency. By converting to polar coordinates (r,ϕ) for which $x = r\cos\phi$ and $y = r\sin\phi$, it is not difficult to show that the differential equation is solved by wavefunctions of the form $\psi_m(\phi,t) = 1/\sqrt{2\pi}\, \exp(im(\phi + \omega t))$, where m must be an integer as is required for the function to be single valued with respect to ϕ at multiples of 2π. The index m indicates that an infinite number of solutions exist; each solution is identified by a unique integer m. The expectation value of the angular momentum along the z axis, $\langle \mathbf{L}_{op,z} \rangle$ for each wavefunction can be found by inserting the wavefunction into the general expectation value equation, with the result $\langle \mathbf{L}_{op,z} \rangle = m\hbar$. Furthermore, the result $\mathbf{L}_{op,z}\psi_m(\phi,t) = m\hbar\psi_m(\phi,t)$ indicates that the wavefunction has well-defined angular momentum given by $\mathbf{L}_z = m\hbar$. Similarly, the expectation value of the energy of each wavefunction is $\langle E_{op} \rangle = -m\hbar\omega$, and the result $E_{op}\psi_m(\phi,t) = -m\hbar\omega\psi_m(\phi,t)$ indicates that the wavefunction has well-defined energy given by $E = -m\hbar\omega$. This quantum mechanical model of the proton correctly predicts that the energy separation of quantum states is $\Delta E = \hbar\omega$. Unfortunately, this model incorrectly predicts an infinite number of energy levels (levels indexed by integer m), rather than just two that are observed experimentally. An adjustment of the representation of angular momentum to a form that represents intrinsic angular moment will yield a proton wavefunction with exactly two energy levels for the magnetic field interaction.

Conversion of space-dependent to <u>intrinsic</u> angular momentum operators

The essential mathematical property of angular momentum operators, which uniquely determine the solution to the differential equation for the wavefunction obeying the angular momentum operator equation, are represented in what is called the operator commutators. The commutator of $\mathbf{L}_{op,x}$ and $\mathbf{L}_{op,y}$ is denoted by the bracket notation $[\mathbf{L}_{op,x}, \mathbf{L}_{op,y}]$ and defined by $[\mathbf{L}_{op,x}, \mathbf{L}_{op,y}] \equiv \mathbf{L}_{op,x}\mathbf{L}_{op,y} - \mathbf{L}_{op,y}\mathbf{L}_{op,x}$. Using the definitions of $\mathbf{p}_{op}$ and $\mathbf{r}_{op}$, the non-zero commutators are found to be $[\mathbf{L}_{op,x}, \mathbf{L}_{op,y}] \equiv i\hbar\mathbf{L}_{op,z}$, $[\mathbf{L}_{op,y}, \mathbf{L}_{op,z}] \equiv i\hbar\mathbf{L}_{op,x}$ and $[\mathbf{L}_{op,z}, \mathbf{L}_{op,x}] \equiv i\hbar\mathbf{L}_{op,y}$. A quantum mechanical point particle with quantized angular momentum can be modeled without assuming a spatial distribution of charge and current, by introducing the concept of intrinsic angular momentum. The intrinsic angular momentum operators will have identical commutation relations to those described above, but no spatial dependence. Let $\mathbf{J}$ denote the quantum mechanical angular momentum based upon the concept of an intrinsic spin $\mathbf{I}$. A set of intrinsic spin operators $\mathbf{I}_{op}$, and intrinsic angular momentum operators $\mathbf{J}_{op}$ that obey the commutation relations are $\mathbf{I}_{op} = \mathbf{\sigma}/2$ and $\mathbf{J}_{op} = \hbar\mathbf{\sigma}/2$, where $\mathbf{\sigma} \equiv (\sigma_x, \sigma_y, \sigma_z)$ are the 2×2 Pauli Spin matrices that obey $[\sigma_x, \sigma_y] \equiv 2i\,\sigma_z$, $[\sigma_y, \sigma_z] \equiv 2i\,\sigma_x$ and $[\sigma_z, \sigma_x] \equiv 2i\,\sigma_y$, and $\mathbf{J}_{op}$ obeys the same commutator equations as $\mathbf{L}_{op}$. Larger dimension

matrices exist that satisfy these commutation relations, but the 2×2 Pauli spin matrices will result in wavefunctions with exactly two energy levels, as needed to match the results of experiments.

Wave equation for the spin ½ proton: The two-component Schrödinger equation

Replacing the angular momentum operator $\mathbf{L}_{op}$ with the intrinsic angular momentum operator $\mathbf{J}_{op}$ in the differential equation derived from $E = -\mathbf{\mu}\cdot\mathbf{B}$, the differential equation becomes $i\hbar\partial\psi(t)/\partial t = -2\pi\gamma_N\hbar(\mathbf{\sigma}/2\cdot\mathbf{B})\psi(t)$, where $\psi(t)$ is a two-component column vector defined by $\psi(t) \equiv \left[\alpha(t)\quad\beta(t)\right]^{\mathrm{T}}$. The vector $\psi(t)$ is referred to as a spinor because it represents the intrinsic properties of the proton that have resulted from the revolving charged particle of the original model. This differential equation is called the two-component Schrödinger Equation. Simplifying and expanding the dot product and all vectors and matrices into their separate components yields

$$\frac{\partial}{\partial t}\begin{bmatrix}\alpha\\\beta\end{bmatrix} = i\pi\gamma\begin{bmatrix}\mathbf{B}_z & \mathbf{B}_x - i\,\mathbf{B}_y\\\mathbf{B}_x + i\,\mathbf{B}_y & -\mathbf{B}_z\end{bmatrix}\begin{bmatrix}\alpha\\\beta\end{bmatrix}$$

It is important to emphasize that by converting to intrinsic angular momentum, the spatial extent of the proton (e.g. radius r) in the original model is lost. However, spatial dependence of the equation and spinor will be introduced through the spatial dependence of the external magnetic fields $\mathbf{B}_x$ $\mathbf{B}_y$ and $\mathbf{B}_z$. The differential equation describes the changes of the proton under the influence of these external magnetic fields and, as detailed below, predicts the evolution of any measurement of a physical parameter such as the proton energy, angular momentum, or magnetic moment.

How spinors determine the observed physical properties of the proton

Expectation values, especially of the proton magnetic moment

The usual computation of the expectation value requires integration over all possible values of the coordinate that the wavefunction was written. For example, in deriving expectation values for wavefunctions $\psi_{n,l,m}(\mathbf{r},t)$ for the hydrogen electron orbitals, integration over all $\mathbf{r}$ would be performed. For the quantum mechanical proton in an external magnetic field, the physical state of the particle at time t is described entirely by just the two values of the spinor, instead of a continuous function of $\mathbf{r}$. Integration over all possible values of the spatial coordinate is replaced by a summation over the two "coordinates" of the vector column. Thus, the expectation value for a general operator, $\mathbf{A}_{op}$ acting on the spinor is a summation over the two components of the spinor:

$$\left\langle\mathbf{A}_{op}\right\rangle = \sum_{j=1}^{2}\psi_j^{\dagger}\left(\mathbf{A}_{op}\psi\right)_j = \alpha^*\left(a_{11}\alpha + a_{12}\beta\right) + \beta^*\left(a_{21}\alpha + a_{22}\beta\right) = \psi^{\dagger}\mathbf{A}_{op}\psi$$

where $\psi_1(t)$ denotes the first component and $\psi_2(t)$ denotes the second component of the spinor $\psi(t)$. The operators of most interest for MRI are those corresponding to the magnetic moment $\mathbf{\mu}$ in each of the three directions, namely: $\mathbf{\mu}_{op,x} = \pi\,\gamma\,\hbar\,\mathbf{\sigma}_x$, $\mathbf{\mu}_{op,y} = \pi\,\gamma\,\hbar\,\mathbf{\sigma}_y$, and $\mathbf{\mu}_{op,z} = \pi\,\gamma\,\hbar\,\mathbf{\sigma}_z$. And inserting each of these in the equation above yields $\left\langle\mathbf{\mu}_{op,x}\right\rangle = \pi\,\gamma\,\hbar\left(\psi^{\dagger}\mathbf{\sigma}_x\psi\right) = 2\pi\,\gamma\,\hbar\operatorname{Re}\left[\alpha^*\beta\right]$, $\left\langle\mathbf{\mu}_{op,y}\right\rangle = \pi\,\gamma\,\hbar\left(\psi^{\dagger}\mathbf{\sigma}_y\psi\right) = 2\pi\,\gamma\,\hbar\operatorname{Im}\left[\alpha^*\beta\right]$, and $\left\langle\mathbf{\mu}_{op,z}\right\rangle = \pi\,\gamma\,\hbar\left(\psi^{\dagger}\mathbf{\sigma}_z\psi\right) = \pi\,\gamma\,\hbar\left(|\alpha|^2 - |\beta|^2\right)$. As for the probability density function, the first component of the spinor gives the probability of the spin 1/2 particle being in the "first" state is given by $|\alpha|^2$, while the probability of finding the spin 1/2 particle in the "second" state is given by $|\beta|^2$. The physical meaning of these different states will become clear upon further analysis of the spinor dynamics. The probability that the spin 1/2 particle is in one or the other state is equal to one, since the particle has to be in one of the available states. This physical requirement is written as: $|\alpha|^2 + |\beta|^2 = 1$.

Protons with well defined magnetic moment

A wavefunction with a "well defined" physical parameter means that a physical system described by that wavefunction will always yield the same measurement in experiments of that physical parameter. If the system is described by a specific two-component spinor with well-defined magnetic moment, then experiments designed to measure the magnetic moment with identically prepared particles will give exactly the same value. A two-component spinor ψ with well-defined magnetic moment will be obey $\mu_{op}\psi = \langle \mu_{op} \rangle \psi$. If the spinor has well-defined energy it will obey $E_{op}\psi = \langle E_{op} \rangle \psi$.

In 1921 Stern and Gerlach conducted an experiment using a beam of silver atoms, in which each silver atom was deflected upward or downward according to whether the magnetic moment that the atom was positive or negative in the direction of a magnetic field spatial gradient. Their experiments showed that the spin 1/2 particles were deflected by the magnetic field gradient to two specific spots (revealed by photographic plate), both equidistant from the center point which corresponded no deflection (and zero magnetic moment). This experiment showed that the magnetic moment of the particles was limited to two values, or quantized.

Stern-Gerlach-type experiments can also be performed with a beam of spin-1/2 protons. The protons can be prepared such that all protons entering the experimental apparatus are in exactly the same quantum mechanical state, i.e., they are represented by the same spinor. The method of preparing these protons is not important for this discussion. The relative number of protons that have positive magnetic moment (i.e., deflected upward and observed at the higher spot on the detector plate) and the relative number that are detected that have negative magnetic moment (i.e., deflected downward and observed at the lower spot on the detector plate) can be derived from the spinor. For example, assume that the Stern-Gerlach apparatus is set up to detect magnetic moment in the *z* direction. If protons are prepared such that 100% will be deflected towards the upper spot, then they are represented by a spinor of the form $\psi = \begin{bmatrix} e^{i\varphi} & 0 \end{bmatrix}^{\mathrm{T}}$ (φ real and arbitrary) which obeys $\mu_{op,z}\psi = \pi\gamma\hbar\psi$ and $\langle \mu_{op,z} \rangle = \pi\gamma\hbar$, $\langle \mu_{op,x} \rangle = \langle \mu_{op,y} \rangle = 0$, and each proton will be measured as having positive magnetic moment in the *z* direction given by $\mu_z = \pi\gamma\hbar$. Similarly, if protons are prepared such that 100% will be deflected towards the lower spot, then they are represented by a spinor of the form $\psi = \begin{bmatrix} 0 & e^{i\varphi} \end{bmatrix}^{\mathrm{T}}$ which obeys $\mu_{op,z}\psi = -\pi\gamma\hbar\psi$ and $\langle \mu_{op,z} \rangle = -\pi\gamma\hbar$, $\langle \mu_{op,x} \rangle = \langle \mu_{op,y} \rangle = 0$, and each proton will be measured as having negative magnetic moment in the *z* direction given by $\mu_z = -\pi\gamma\hbar$. As a second example, say that the Stern-Gerlach apparatus is rotated to detect magnetic moment in the *y* direction. If protons are prepared in a quantum mechanical state that results in 100% of the protons being deflected to the upper spot, then they are represented by a spinor of the form $\psi = 1/\sqrt{2}\begin{bmatrix} e^{i\varphi} & i\,e^{i\varphi} \end{bmatrix}^{\mathrm{T}}$ (φ real and arbitrary) which obeys $\mu_{op,y}\psi = \pi\gamma\hbar\psi$ and $\langle \mu_{op,y} \rangle = \pi\gamma\hbar$ and $\langle \mu_{op,x} \rangle = \langle \mu_{op,z} \rangle = 0$, and each proton will be measured as having a positive magnetic moment in the *y* direction $\mu_y = \pi\gamma\hbar$. Similarly, if protons are prepared so that 100% will deflect towards the lower spot, then they are represented by a spinor of the form $\psi = 1/\sqrt{2}\begin{bmatrix} e^{i\varphi} & -i\,e^{i\varphi} \end{bmatrix}^{\mathrm{T}}$ which obeys $\mu_{op,y}\psi = -\pi\gamma\hbar\psi$ and $\langle \mu_{op,y} \rangle = -\pi\gamma\hbar$, $\langle \mu_{op,x} \rangle = \langle \mu_{op,z} \rangle = 0$, and each proton is measured as having a negative magnetic moment in the *y* direction $\mu_y = -\pi\gamma\hbar$.

A general spinor of the form $\psi = \begin{bmatrix} \alpha & \beta \end{bmatrix}^{\mathrm{T}}$ will in general not have well-defined angular momentum in any of the *orthogonal* directions *x, y* or *z*. However, for this spinor there is a particular direction for which the protons have well-defined magnetic moments. In other words, an orientation of the Stern Gerlach apparatus can be found so that 100% of the protons will be deflected to the upper spot, or the lower spot of the detection plate. We consider the magnetic moment operator $\mu_{op,\hat{n}} = \pi\gamma\hbar(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})$ for the direction $\hat{\mathbf{n}}$ given by the spherical coordinate angles θ,φ: $\hat{\mathbf{n}} = \begin{bmatrix} \sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta \end{bmatrix}$. The equation $\mu_{op,\hat{\mathbf{n}}}\psi = \pi\gamma\hbar\psi$ defines a spinor having well-defined positive magnetic moment along the direction $\hat{\mathbf{n}}$. This equation can be simplified to $(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})\psi = \psi$. Given α and β, θ,φ defining $\hat{\mathbf{n}}$, and ϕ defining the overall phase, the spinor can be determined implicitly from $\alpha = \exp i\phi \cos\theta/2$ and $\beta = \exp i(\phi+\varphi)\sin\theta/2$. The equation $(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})\psi = -\psi$ defines a spinor having well-defined *negative* magnetic

moment along the direction $\hat{\mathbf{n}}$. This direction can be determined implicitly from $\alpha = -\exp i\left(\phi-\varphi\right)\sin\theta/2$ and $\beta = \exp i\,\phi\cos\theta/2$.

Probability of a proton being detected spin-up or spin-down

To know the probability that a proton will contribute a positive or negative magnetic moment along a direction $\hat{\mathbf{n}}$, the general spinor must be decomposed into a sum of spinors representing protons that are spin-up and spin-down along direction $\hat{\mathbf{n}}$. This decomposition is $\psi = a_{\mathbf{n}}\left[\cos\theta/2 \quad \exp i\varphi\sin\theta/2\right]^{\mathrm{T}} + b_{\mathbf{n}}\left[-\exp\left(-i\varphi\right)\sin\theta/2 \quad \cos\theta/2\right]^{\mathrm{T}}$, from which it is found for a given spinor $\psi = \left[\alpha \quad \beta\right]^{\mathrm{T}}$, $a_{\mathbf{n}} = \alpha\cos\theta/2 + \beta\exp\left(-i\,\varphi\right)\sin\theta/2$ and $b_{\mathbf{n}} = \beta\cos\theta/2 - \alpha\exp\left(-i\,\varphi\right)\sin\theta/2$. Accordingly, $\left|a_{\mathbf{n}}\right|^2$ is the probability that the proton will be detected with positive magnetic moment (spin-up) in the direction $\hat{\mathbf{n}}$, and $\left|b_{\mathbf{n}}\right|^2$ is the probability that the proton will be detected with negative magnetic moment (spin-down) along direction $\hat{\mathbf{n}}$. This formula can also be used to determine the probability of detecting the spinor $\psi = \left[\alpha \quad \beta\right]^{\mathrm{T}}$ as spin-up or spin down in any of the orthogonal directions, using $\left(\theta,\varphi\right) = \left(0,0\right)$ for the z direction, $\left(\theta,\varphi\right) = \left(\pi/2,0\right)$ for the x direction, and $\left(\theta,\varphi\right) = \left(\pi/2,\pi/2\right)$ for the y direction.

MRI measures the expectation value of the magnetic moment of the protons

In MRI, the RF coil detects the rapidly changing magnetization vector $\mathbf{M}$ of the tissue according to the reciprocity formula $\zeta = -\partial/\partial t\left(\mathbf{M}\cdot\hat{\mathbf{B}}_1\right)$ where ζ is the induced voltage in the coil, and $\hat{\mathbf{B}}_1$ is the reference field of the RF coil. The transverse and longitudinal components of the magnetization vector $\mathbf{M}$ are proportional to the corresponding expectation values for the magnetic moments: $\mathbf{M}_x + i\,\mathbf{M}_y \equiv n_0\left(\left\langle\boldsymbol{\mu}_{op,x}\right\rangle + i\left\langle\boldsymbol{\mu}_{op,y}\right\rangle\right)$, $\mathbf{M}_z \equiv n_0\left\langle\boldsymbol{\mu}_{op,z}\right\rangle$, where n_0 is the excess number of protons at thermal equilibrium that, if measured, would be measured with positive magnetic moment along the direction of the main magnetic field. The RF coil detects the expectation value of the spinor representing the quantum mechanical protons in the tissue. Each voxel of tissue will have a collection of protons that are in the same quantum mechanical state. i.e., each of the protons in the collection are described by the same spinor (to within an overall phase angle). As in the Stern-Gerlach experiments, each proton is detected with either a positive or negative unit of magnetic moment. However, unlike the process of the Stern-Gerlach experiment, in MRI, the protons within each voxel are not measured one-by-one. At any instant of time, only the entire collection of protons is measured as an induced voltage ζ in the RF coil. If, for example, the protons have 50% probability of being detected with positive magnetic moment along the axis of sensitivity of the RF coil (determined at each voxel by the reference field), and 50% probability of being detected with negative magnetic moment, then no magnetic moment is detected, and no voltage is generated in the RF coil. In a large collection of identically-prepared protons, the total induced voltage will be proportional to the number of positive magnetic moments measured, minus the number of negative magnetic moments measured. The positive contribution to the voltage is equal to the probability of the proton being measured with positive magnetic moment, multiplied by the total number of protons measured and the unit magnetic moment of the proton. A similar statement is valid for the negative contribution to the voltage. Although the magnetic moment of each proton is quantized, the magnetization, which is the result of a summation from a large collection of protons, has a continuum of values. Because of the large number of protons contributing magnetic moment, the magnetization vector is not observed as being quantized.

Two examples of solutions of the two-component Schrödinger equation

Precession

The values of α and β can be changed by changing the magnetic fields $\mathbf{B}_x$, $\mathbf{B}_y$ (the RF field) and $\mathbf{B}_z$ (the main field and field gradients). Precession occurs in the presence of a main magnetic field and no RF field. The Schodinger equation simplifies to a diagonal matrix with $\mathbf{B}_z \neq 0$ and $\mathbf{B}_x = \mathbf{B}_y = 0$.

$$\frac{\partial}{\partial t}\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} i\pi\gamma\mathbf{B}_z & 0 \\ 0 & -i\pi\gamma\mathbf{B}_z \end{bmatrix}\begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

The solution to this differential equation is $\alpha(t) = \alpha(0)\exp(i\pi\gamma\mathbf{B}_z t)$ and $\beta(t) = \beta(0)\exp(-i\pi\gamma\mathbf{B}_z t)$, where $\alpha(0)$ and $\beta(0)$ are initial conditions. The magnetization derived from the expectation values is as follows: $\mathbf{M}_z = |\alpha(0)|^2 - |\beta(0)|^2$ and $\mathbf{M}_x + i\mathbf{M}_y \equiv 2\alpha^*(0)\beta(0)\exp(-i2\pi\gamma\mathbf{B}_z t)$. Note that the overall factor of $\mathbf{M}_0 \equiv n_0\pi\gamma\hbar$, the thermal equilibrium magnetization that multiplies each component of $\mathbf{M}$, is set equal to 1. This simplification is done for the convenience of not having to write this factor each time. These magnetization equations reveal that the z magnetization is constant and that the transverse magnetization rotates according to the "left-hand rule" at the Larmor frequency given by $2\pi\gamma\mathbf{B}_z t$. The rotation around the axis of the main magnetic field is referred to as precession. The left-hand rule states that when the thumb of the left-hand is aligned along the axis of the applied magnetic field, the direction of the curl of the fingers defines the rotation of the magnetization vector.

Nutation

In MRI, the main magnetic field is defined to be along the z axis, and RF pulses are applied in the transverse plane as additional, rapidly time-varying magnetic fields. The dynamics of the spinor and of the magnetization vector are affected by both fields. When an RF pulse is applied, longitudinal magnetization vector is rotated toward the transverse plane, a process called nutation. The mathematical representation of nutation is accomplished by transforming the Schrödinger equation into a rotating reference frame. A magnetization vector precessing at the Larmor frequency in the laboratory frame appears to be stationary in the rotating frame, with fixed angles between the vector and the rotating frame x and y axes. After the Schrödinger equation is transformed to the rotating reference frame, often the dynamics of spinor is simpler and can be solved. This solution can then be transformed back into the laboratory frame. With initial spinor corresponding to protons that are spin-up in the z direction (this spinor is the same in both laboratory and rotating frames), the spinor for the laboratory frame under the action of a main magnetic field and an RF field (y direction) with amplitude B_1 and temporal frequency $2\pi\gamma\mathbf{B}_z t$ is given by $\alpha(t) = \cos(\pi\gamma|B_1|t)\exp(i\pi\gamma\mathbf{B}_z t)$ and $\beta(t) = -\sin(\pi\gamma|B_1|t)\exp(-i\pi\gamma\mathbf{B}_z t)$, and the magnetization components derived from the expectation values are $\mathbf{M}_x + i\mathbf{M}_y = -\sin(2\pi\gamma|B_1|t)\exp(2i\pi\gamma\mathbf{B}_z t)$ and $\mathbf{M}_z = \cos(2\pi\gamma\mathbf{B}_z t)$. These equations describe a magnetization vector that precesses around the z axis as it is being rotated down toward the transverse plane from the z axis.

From the Schrödinger equation to the Bloch equation

Origin of the off-diagonal terms describing magnetization vector rotations

The Bloch Equation without relaxation and recovery terms is a differential equation for the evolution of the expectation values of the single proton magnetic moment. It is determined by taking the time derivative of the expectation value equations. For example, with $\mathbf{M}_x = \psi^\dagger\boldsymbol{\sigma}_x\psi$, $\partial\mathbf{M}_x/\partial t = (\partial\psi^\dagger/\partial t)\boldsymbol{\sigma}_x\psi + \psi^\dagger\boldsymbol{\sigma}_x(\partial\psi/\partial t)$, with similar equations for $\mathbf{M}_y$ and $\mathbf{M}_z$. Using the Schrödinger equation and the commutation relations between $\boldsymbol{\sigma}_x$, $\boldsymbol{\sigma}_y$, and $\boldsymbol{\sigma}_z$ to simplify and apply to all combinations of $\mathbf{B}$, and repeating the process for $\mathbf{M}_y$ and $\mathbf{M}_z$, the individual equations of the Bloch equation without relaxation and recovery terms can be written as $\partial\mathbf{M}_x/\partial t = 2\pi\gamma\mathbf{B}_z\mathbf{M}_y - 2\pi\gamma\mathbf{B}_y\mathbf{M}_z$, $\partial\mathbf{M}_y/\partial t = 2\pi\gamma\mathbf{B}_x\mathbf{M}_z - 2\pi\gamma\mathbf{B}_z\mathbf{M}_x$ and $\partial\mathbf{M}_z/\partial t = 2\pi\gamma\mathbf{B}_y\mathbf{M}_x - 2\pi\gamma\mathbf{B}_x\mathbf{M}_y$. In standard 3×3 matrix form, these are

$$\frac{\partial}{\partial t}\begin{bmatrix} \mathbf{M}_x \\ \mathbf{M}_y \\ \mathbf{M}_z \end{bmatrix} = 2\pi\gamma\begin{bmatrix} 0 & \mathbf{B}_z & -\mathbf{B}_y \\ -\mathbf{B}_z & 0 & \mathbf{B}_x \\ \mathbf{B}_y & -\mathbf{B}_x & 0 \end{bmatrix}\begin{bmatrix} \mathbf{M}_x \\ \mathbf{M}_y \\ \mathbf{M}_z \end{bmatrix}$$

In this form, the Bloch equation is a differential equation for rotations in three-dimensional space. The magnetization vector represents the expectation value of the magnetic moment and is rotated by the action of the external magnetic fields according to the "left-hand rule".

Origins of decay, recovery and thermal equilibrium magnetization terms

Theory of exchange between spin system and reservoir (the tissue lattice)

When a spin transitions from the high energy state to the low energy state, a reservoir in thermal contact (capable of exchanging energy) with the spin system must possess a quantum mechanical state that can transition to a higher energy state. This transition rate (i.e., transitions per second) per spin is denoted $W_\downarrow = N_b W_{-b\to+a}$. where N_b denotes the number of states in the reservoir that can accept a quanta of energy, and $W_{-b\to+a}$ is the transition rate per spin per reservoir state. Similarly, for the opposite transfer of energy, the availability of a quantum mechanical state in the reservoir to transition to a lower energy state is necessary. This transition rate per spin is denoted $W_\uparrow = N_a W_{+a\to-b}$, where N_a denotes the number of states in the reservoir that can release a quanta of energy, and $W_{+a\to-b}$ is the transition rate per spin per reservoir state. An essential postulate of statistical mechanics, applied at the deepest point of this model (deepest meaning that the defined particles and states of the system at that level are not further dissected) is the postulate of microscopic reversibility. For this model, this postulate is expressed as $W_{-b\to+a} = W_{+a\to-b}$. Under these conditions, a spin system initially with equal numbers of spins in the low and high energy state will develop a net excess of spins in the lower energy state, according to the differential equation $dn/dt = W_\downarrow (N - n) - W_\uparrow (N + n)$, where $N = N_+ - N_-$ is the total number of spins in the volume, N_+ and N_- are the number in the low and high energy state, respectively, and $n = N_+ - N_-$ is the excess of spins in the low energy state. The form of this differential equation which defines the longitudinal relaxation time T_1 and thermal equilibrium magnetization n_0 is $dn/dt = (n_0 - n)/T_1$, where $n_0 = N\left((W_\downarrow - W_\uparrow)/(W_\downarrow + W_\uparrow)\right)$ and $T_1 = 1/(W_\downarrow + W_\uparrow)$. For example, taking $n(0) = 0$, the solution of this differential equation is $n(t) = n_0 (1 - \exp(-t/T_1))$. Recalling that $\mathbf{M}_z = \pi \gamma \hbar n$, the excess number of spin-up protons times the magnetic moment of a single proton, we see that the solution describes T_1 recovery of longitudinal magnetization towards the thermal equilibrium magnetization given by $\mathbf{M}_0 = \pi \gamma \hbar n_0$.

Derivation of the Boltzmann equation

While the model above predicts the possibility of an excess of spin-up protons if there is a mechanism for energy exchange between the spin system and the lattice, the model does not determine actual numerical values for this excess. Deriving numerical values requires the concept that the observed partition of energy between two physical systems in thermal contact with other corresponds to the partition that yields the greatest number of assessable states. Any particular quantum mechanical configuration of the spin system and lattice state has equal chance of being the observed state of the physical system. A "configuration" of the spin system is defined as the collection of spins that are spin-up and those that are spin-down, with all spins uniquely identified. A configuration of the lattice is defined as the collection of quantum mechanical states of the tissue lattice, e.g., collectively all quantum-mechanical vibrational, translational and rotational states of the tissue macromolecules and small molecules, with each state uniquely identified. Each spin system configuration and lattice configuration with the correct total energy has an equal chance of being the observed state of the physical system. The physical system moves very rapidly through all different spin system and lattice configurations which are consistent with the total energy of the combined system. The observed energy partition is simply the one associated with the greatest number of available spin system configurations and lattice configurations.

Define $g_s(N_s, E_s)$ as the number of states available in the spin system composed of N_s protons and energy E_s. Similarly, define $g_r(N_r, E_r)$ as the number of states available only in the reservoir (tissue lattice) composed of N_r particles and energy E_r. For any particular distribution of the total energy, the total number of available states available, denoted $g(N_s, N_r, E_s, E_r) = g_s(N_s, E_s) g_r(N_r, E_r)$, is the product of the number of states available

in the spin system times the number available in the reservoir. Thermal equilibrium is defined by the condition that $g\left(N_s, N_r, E_s, E_r\right)$ is maximized by exchanging energy (particles are not exchanged), or equivalently, when $\partial g/\partial E_s = 0$. The zero derivative condition can be written $g_s\left(E_s\right)/g_s\left(E_s + \Delta E_s\right) = g_r\left(E_r - \Delta E_s\right)/g_r\left(E_r\right)$, with $\Delta E_s = 2\pi\gamma\hbar\mathbf{B}_0$. N_s and N_r are not listed as arguments because they are not exchanged. Using combinatorics to count the spin states yields $g_s\left(E_s\right)/g_s\left(E_s + \Delta E_s\right) = N_-^0/N_+^0$, where N_-^0 and N_+^0 are the number of spin-down (high energy) and spin-up (low energy) protons, respectively, at thermal equilibrium. Using a collection of non-interacting particles carrying kinetic energy as a model of the lattice yields $g_r\left(E_r - \Delta E_s\right)/g_r\left(E_r\right) = \exp\left(-\Delta E_s/kT\right)$. Combining using the zero derivative condition yields the Boltzmann equation $N_-^0/N_+^0 = \exp\left(-\Delta E_s/kT\right)$.

Decay and recovery terms

The term T_2 models the decay of transverse magnetization $\left(\mathbf{M}_x, \mathbf{M}_y\right)$, and the term T_1 models the decay of longitudinal magnetization $\mathbf{M}_z$, as well as recovery of longitudinal magnetization towards the thermal equilibrium magnetization caused by energy exchange with the tissue lattice. These terms can be derived from models of physical effects that destroy the condition that all protons within a voxel are in the same quantum mechanical state, i.e., are represented by the same spinor. The gradual loss of similarity of spinors representing the protons is referred to as a loss of coherency of the quantum mechanical system. The loss of coherency of the system is an inevitable process caused by differences of the local microscopic magnetic field environment of the different protons in the tissue. T_1 and T_2 can be calculated for different tissues using a statistical model of these time-varying microscopic magnetic fields affecting individual protons. Using first and second order statistics, the correlation time, power spectrum, and variance of the random time-varying magnetic fields can be calculated. Using this model, loss of longitudinal magnetization is given by $\mathbf{M}_z(t) = \mathbf{M}_z(0)\exp\left(-\tfrac{1}{2}\left(\sigma_{\phi_x}^2(t) + \sigma_{\phi_y}^2(t)\right)\right)$, where $\sigma_{\phi_x}^2(t)$ and $\sigma_{\phi_y}^2(t)$ are time-dependent variances of the angular spread of the expectation values induced by action of random microscopic magnetic fields in the x and y direction, repectively. The loss of transverse magnetization is given by $\mathbf{M}_x(t) = \mathbf{M}_x(0)\exp\left(-\tfrac{1}{2}\left(\sigma_{\phi_z}^2(t) + \sigma_{\phi_x}^2(t)\right)\right)$ and $\mathbf{M}_y(t) = \mathbf{M}_y(0)\exp\left(-\tfrac{1}{2}\left(\sigma_{\phi_z}^2(t) + \sigma_{\phi_x}^2(t)\right)\right)$, where $\sigma_{\phi_z}^2(t)$ is the variance of the angular spread of the transverse expectation values induced by action of random magnetic fields in the z direction. Based on the Schrödinger equation, the spread of expectation values in the presence of random magnetic fields with zero mean and variances $\sigma_{\mathbf{B}_\perp}^2 \equiv \sigma_{\mathbf{B}_x}^2 = \sigma_{\mathbf{B}_y}^2$ and $\sigma_{\mathbf{B}_z}^2$, and correlation times of τ_0, is given by $\sigma_{\phi_x}^2 = \sigma_{\phi_y}^2 = 2(2\pi\gamma)^2 \sigma_{\mathbf{B}_\perp}^2 \tau_0 t / \left(1 + \omega^2\tau_0^2\right)$ and $\sigma_{\phi_z}^2 = 2(2\pi\gamma)^2 \sigma_{\mathbf{B}_z}^2 \tau_0 t$. Simple identification of $1/T_1$ and $1/T_2$ in the exponents of the magnetization equations yields the following widely accepted equations for $1/T_1$ and $1/T_2$:
$1/T_1 = 2(2\pi\gamma)^2 \sigma_{\mathbf{B}_\perp}^2 \tau_0 / \left(1 + \omega^2\tau_0^2\right)$ and $1/T_2 = (2\pi\gamma)^2 \left(\sigma_{\mathbf{B}_z}^2 \tau_0 + \sigma_{\mathbf{B}_\perp}^2 \tau_0 / \left(1 + \omega^2\tau_0^2\right)\right)$.

The Bloch Equation

By combining contributions to the time derivatives of the magnetic moment expectation values from (1) the two-component Schrödinger equation describing the dynamics of a single proton, (2) the recovery of longitudinal magnetization based on energy exchange between the spin system with the lattice and (3) the decay of magnetization due to the action of microscopic random magnetic fields, the complete Bloch Equation is obtained:

$$\frac{\partial}{\partial t}\begin{bmatrix}\mathbf{M}_x \\ \mathbf{M}_y \\ \mathbf{M}_z\end{bmatrix} = \begin{bmatrix}-1/T_2 & 2\pi\gamma\mathbf{B}_z & -2\pi\gamma\mathbf{B}_y \\ -2\pi\gamma\mathbf{B}_z & -1/T_2 & 2\pi\gamma\mathbf{B}_x \\ 2\pi\gamma\mathbf{B}_y & -2\pi\gamma\mathbf{B}_x & -1/T_1\end{bmatrix}\begin{bmatrix}\mathbf{M}_x \\ \mathbf{M}_y \\ \mathbf{M}_z\end{bmatrix} + \begin{bmatrix}0 \\ 0 \\ \mathbf{M}_0/T_1\end{bmatrix}$$

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